Molecular Dynamics Simulation of Coherent Interfaces in Fluorite Heterostructures: Supplementary Information

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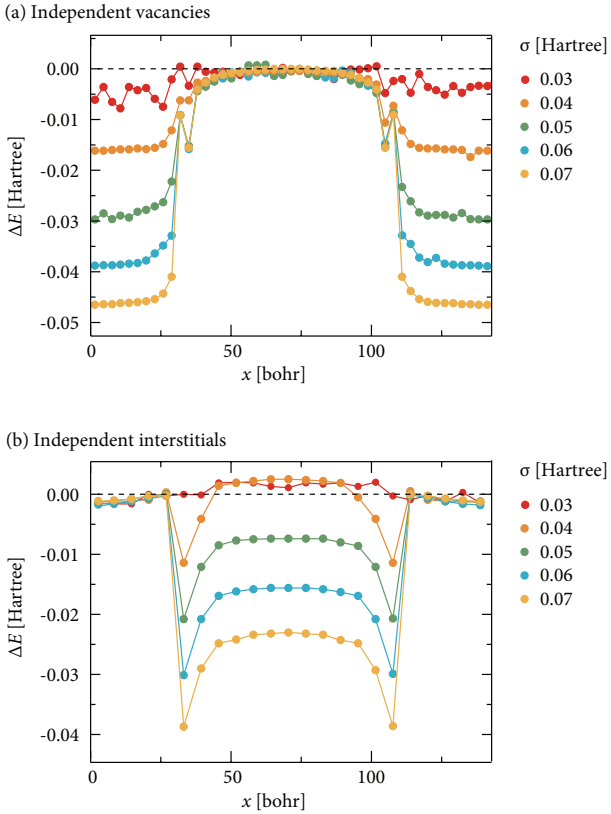

FIG. S1: Defect formation energies for single vacancies and interstitials as a function of x for $\sigma_{\mathrm{F}} = 0.04, 0.05, 0.06, 0.07$.

Fig. S1 plots relative energies as a function of σ_{F} for independent vacancies (upper panel) and interstitials (lower panel) at all possible x-positions in the simulation cell with fully relaxed geometries.

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